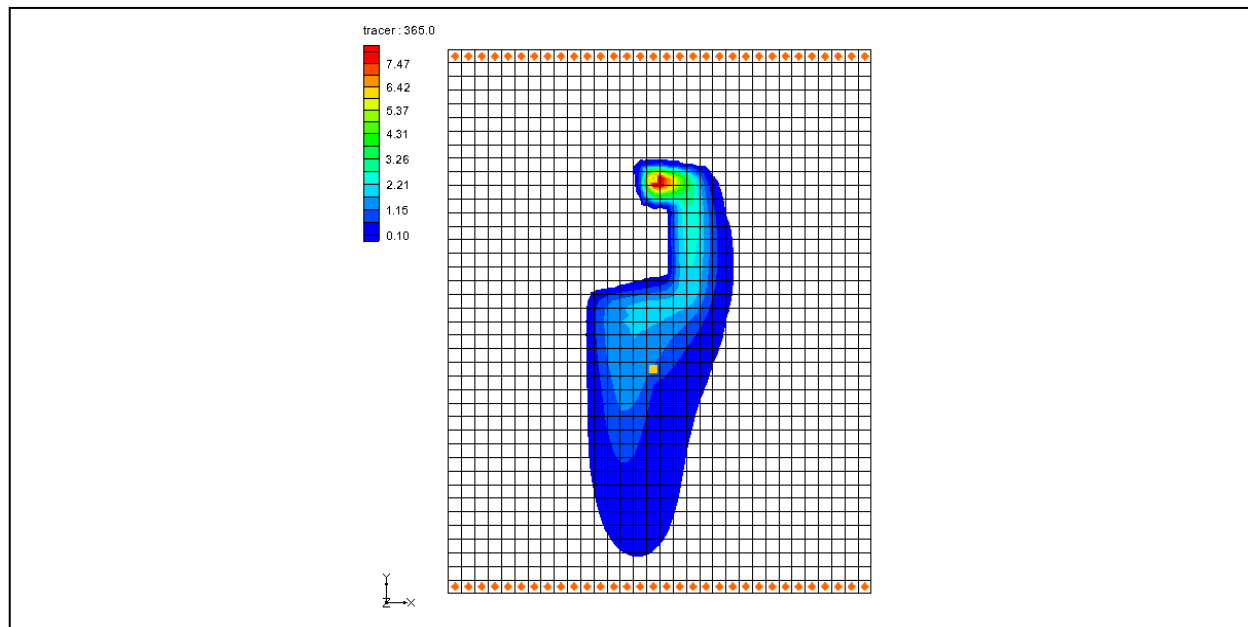


GMS 10.0 Tutorial

MT3DMS – Grid Approach

Create an MT3DMS model using the grid approach



Objectives

Construct a MT3DMS model using the grid approach. Values are manually assigned to the grid. Simple models can be easily constructed using the grid approach.

Prerequisite Tutorials

- MODFLOW – Grid Approach

Required Components

- Grid Module
- MODFLOW
- MT3DMS

Time

- 15-25 minutes



1	Introduction	2
1.1	Outline.....	2
2	Description of Problem	2
3	Getting Started	3
4	The Flow Model	3
5	Building the Transport Model	4
5.1	Initializing the Simulation.....	4
5.2	The Basic Transport Package.....	5
5.3	The Advection Package.....	6
5.4	The Dispersion Package.....	6
5.5	The Source/Sink Mixing Package.....	7
5.6	Saving the Simulation and Running MT3DMS.....	7
5.7	Changing the Contouring Options.....	8
5.8	Setting Up an Animation.....	8
5.9	Calculating the Mass of the Contaminant.....	8
6	Conclusion	9

1 Introduction

This tutorial describes how to perform an MT3DMS simulation within GMS. An MT3DMS model can be constructed in GMS using one of two approaches: the conceptual model approach or the grid approach. With the conceptual model approach, the sources/sinks and zones in the model are defined with GIS objects and automatically assigned to the grid. With the grid approach, values are manually assigned to the grid. While the conceptual model approach is generally preferable for large, complicated models, simple models can be easily constructed using the grid approach. The grid approach is described in this tutorial.

1.1 Outline

Here are the steps for this tutorial:

1. Open a MODFLOW simulation and run MODFLOW.
2. Initialize MT3D and enter the data for several MT3D packages.
3. Run MT3D and read the solution.
4. Set up an animation to visualize the solution.
5. Calculate the mass of the contaminant.

2 Description of Problem

The problem in this tutorial is shown in Figure 1. This problem corresponds to the sixth sample problem (“Two-Dimensional Transport in a Heterogeneous Aquifer”) described in the MT3DMS documentation. The problem consists of a low K zone inside a larger zone. The sides of the region are no flow boundaries. The top and bottom are constant

head boundaries that cause the flow to move from the top to the bottom of the region. An injection well with a specified concentration provides the source of the contaminants. A pumping well serves to withdraw contaminated water migrating from the injection well. A steady state flow solution will be computed and a transient transport simulation will be performed over a one year period.

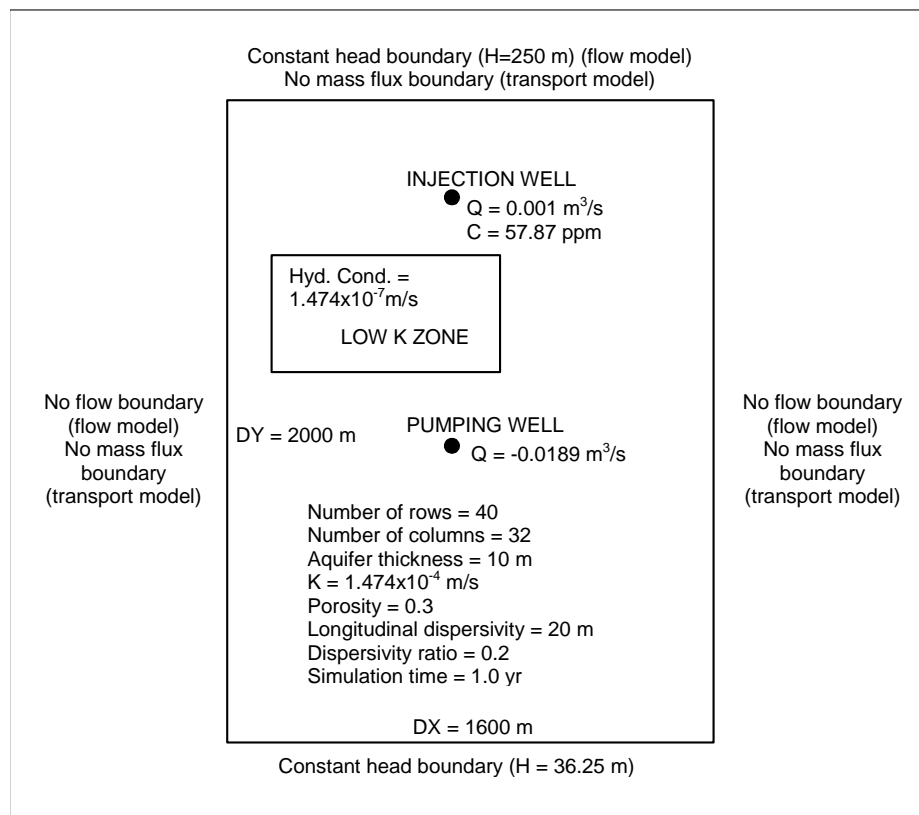


Figure 1 Sample flow and transport problem


3 Getting Started

Do the following to get started:


1. If necessary, launch GMS.
2. If GMS is already running, select the *File / New* command to ensure that the program settings are restored to their default state.

4 The Flow Model

Before setting up the MT3DMS simulation, the user must first have a MODFLOW simulation. The MODFLOW solution will be used as the flow field for the transport simulation. In the interest of time, the user will read in a previously created MODFLOW simulation.

1. Select the **Open**  button.
2. Locate and open the directory entitled *Tutorials\MT3D\mt3dgrid*.
3. Select the file entitled “flowmod.gpr.”
4. Click **Open**.

Now the user will save the project under a new name. Since the user is changing the name, the user will run MODFLOW to compute solution files with the new name. Otherwise, when MT3D runs, it will look for solution files with the new name and not find any.


5. Select the *File* | **Save As** command.
6. Locate and open the directory entitled *Tutorials\ MT3D\mt3dgrid*.
7. Change the project name to “transport.gpr.”
8. Click **Save**.
9. Select the “3D Grid Data” folder from the Project Explorer.
10. Click the **Run MODFLOW**  button.
11. When it finishes running, select the **Close** button.

5 Building the Transport Model

Now that the user has a flow solution, it is possible to set up the MT3DMS transport simulation. Like MODFLOW, MT3DMS is structured in a modular fashion and uses a series of packages as input. Consequently, the GMS interface to MT3DMS is similar to the interface to MODFLOW, and the user will follow a similar sequence of steps to enter the input data.

5.1 Initializing the Simulation

First, initialize the MT3DMS simulation.

1. Expand the “3D Grid Data” folder.
2. Right-click on the “grid”  item in the Project Explorer.
3. Select the **New MT3D...** command to open the *Basic Transport Package* dialog.

5.2 The Basic Transport Package

The MT3DMS Basic Transport Package dialog is always required, and it defines basic information such as stress periods, active/inactive regions, and starting concentration values.

Species

Since MT3DMS is a multi-species model, it is necessary to define the number of species and name each species. The user will use one species named “tracer.”

1. Select the **Define Species** button to open the *Define Species* dialog.
2. Select the **New** button.
3. Change the name of the species to “tracer.”
4. Select the **OK** button.

Packages

Next, select which packages to use.

1. Select the **Packages** button to open the *MT3D/RT3D Packages* dialog.
2. Turn on the following packages:
 - *Advection Package*
 - *Dispersion Package*
 - *Source/Sink Mixing Package*
3. Select the **OK** button.

Stress Periods

The next step is to set up the stress periods. The flow simulation was steady state but the transport simulation will be transient. The user will run the simulation for a one-year time period. To do this, the user will use a single stress period (since the input values are constant) and allow MT3DMS to determine the appropriate transport step size.

1. Select the **Stress Periods** button to open the *Stress Periods* dialog.
2. In the first row, change the *Length* field to “365.”
3. Make sure the value in the *Trans. step size* is “0.0.” A value of zero signifies that MT3DMS will automatically compute the appropriate transport step size.
4. Select the **OK** button to exit the *Stress Periods* dialog.

Output Control

Next, specify the output options.

1. Select the *Output Control* button to open the *Output Control* dialog.
2. Select the *Print or save at specified interval* option.
3. Change the specified interval to “10.” This will output a solution at every tenth transport step.
4. Select the **OK** button to exit the *Output Control* dialog.

ICBUND Array

The ICBUND array is similar to the IBOUND array in MODFLOW. The ICBUND array is used to designate active transport cells (ICBUND>0), inactive transport cells (ICBUND=0), and constant concentration cells (ICBUND<0). For this problem, all of the cells are active, therefore, no changes are necessary.

Starting Concentration Array

The starting concentration array defines the initial condition for the contaminant concentration. In the current problem, the starting concentrations are all zero, so the default is adequate.

HTOP and Thickness Arrays

MT3DMS uses the HTOP array and a thickness array to determine the layer geometry. However, the values for these arrays are determined by GMS automatically from the MODFLOW layer data, so no input is necessary.

Porosity Array

Finally, the user will define the porosity for the cells. This problem has a constant porosity of 0.3. This is the default value in GMS, so no changes need to be made.

This completes the definition of the Basic Transport package data.

1. Select the **OK** button to exit the *Basic Transport Package* dialog.

5.3 The Advection Package

The next step is to enter the data for the Advection package. This tutorial will use the *Third Order TVD scheme (ULTIMATE)* solution scheme. This is the default, so nothing needs to be done.

5.4 The Dispersion Package

Next, enter the data for the Dispersion package.

1. Select the *MT3DMS* | **Dispersion Package** command to open the *Dispersion Package* dialog.
2. Select the **Longitudinal Dispersivity** button.
3. Select the **Constant** → **Grid** option to open the *Grid Value* dialog.
4. Enter a value of “20.”
5. Click **OK**.
6. Select the **OK** button to exit the *Longitudinal Dispersivity* dialog.
7. Enter a value of “0.2” for the *TRPT* parameter.
8. Select the **OK** button to exit the *Dispersion Package* dialog.

5.5 The Source/Sink Mixing Package

Finally, the user must define the data for the Source/Sink Mixing package. For this problem, the user only has one source/sink: the injection well. To define the source at the injection well, the user needs to select the well and assign a concentration.

1. Select the cell containing the injection well (the upper well) by clicking anywhere in the interior of the cell.
2. Right-click on the selected cell.
3. Select the **Sources/Sinks** menu command.
4. On the left side of the dialog, select the *MT3D: Point SS* item.
5. Click the **Add BC** button near the bottom of the dialog.
6. Change the *Type (ITYPE)* to “well (WEL).”
7. Enter “57.87” for the concentration in the *tracer* column.
8. Select the **OK** button to exit the dialog.
9. Click outside the grid to unselect the cell.

5.6 Saving the Simulation and Running MT3DMS


The user is now ready to save the simulation and run MT3DMS.

1. Select the **Save**  button.
2. Select the **Run MT3D**  button.

3. When the simulation is finished, select the **Close** button.

5.7 Changing the Contouring Options

When displaying plume data, the color fill option often provides excellent results.



1. Click on the **Contour Options**  button to open the *Dataset Contour Options – 3D Grid – tracer* dialog.
2. Change the *Contour method* to “Color Fill.”
3. Select the **OK** button.

5.8 Setting Up an Animation

Now the user will observe how the solution changes over the one-year simulation by generating an animation. Do the following to set up the animation:

1. Select the *Display / Animate* command.
2. Make sure the *Data set* option is on.
3. Click **Next**.
4. Turn on the *Display clock* option.
5. Select the *Use constant interval option*.
6. Change the *Time interval* to “36.5.” This will result in 11 frames.
7. Select the **Finish** button.

The user should see some images appear on the screen. These are the frames of the animation which are being generated.

8. After viewing the animation, select the **Stop**  button to stop the animation.
9. Select the **Step**  button to move the animation one frame at a time.
10. The user may wish to experiment with some of the other playback controls. When finished, close the window and return to GMS.

5.9 Calculating the Mass of the Contaminant

Finally, the user will calculate the mass of the contaminant in the aquifer at various times during the simulation.

1. Choose the **Select Cells**  tool.

2. Select the cell containing the well in the lower portion of the model.
3. Select the *MT3DMS* / **Calculate Mass** command to open the *Calculate Mass* dialog.

This dialog allows the user to calculate the mass of a contaminant in the entire model domain or in the selected cell(s). The *Definition* section of the dialog explains the formula that is used to calculate the mass. Basically, the volume of water in each cell is calculated and then multiplied by the concentration computed by MT3D. The user must supply a conversion factor so that the calculated mass will be computed in the correct units. The *Unit conversion factor* section shows an example of a conversion factor. The *Concentration range* section allows the user to specify a range over which the mass will be calculated. This is most useful to ignore negative concentrations that result in MT3D simulations.

4. In the *Concentration range* section, turn on the *Specify range in calculation* toggle.
5. Enter “0.0” for the *Min*.
6. Enter “9.0” for the *Max*.
7. In the *Unit conversion factor* section, enter “0.0283” for the *Factor* so that the resulting mass will be in units of grams.
8. Select the *Use only selected cells in calculation* option near the bottom of the dialog.
9. Select the **Calculate** button.

Notice that the mass values are shown in the spreadsheet on the right side of the dialog.

10. Now select the *Use all cells in calculation* option.
11. Select the **Calculate** button again.

The user should now see the total mass in the aquifer for each time step of the solution.

12. When finished viewing the results, select **Done** to close the dialog

6 Conclusion

This concludes the “MT3DMS – Grid Approach” tutorial. Here are key concepts in this tutorial:

- MT3D is available only if a MODFLOW model is in memory.

- MT3D relies on the MODFLOW solution files, so if MODFLOW files are moved or renamed, the user will probably need to regenerate the MODFLOW solution files so that MT3D can find them.
- GMS gives MT3D the top and bottom elevation data it requires for each layer from the MODFLOW model.
- It is possible to use the *Animation Wizard* to create an animation in GMS.
- It is possible to calculate the mass of a contaminant in the 3D grid using the *MT3D / Calculate Mass* command.